[redacted] **Final** **FOCUS REPORT**
New Chemicals Program

PART I: BACKGROUND

Written By: DHN

FOCUS DATE: 6/14/2007 **FOCUS CHAIR:** J. Alwood

COMPANY: [redacted]

CASE NUMBER(S): P07-0467 **through** **and**

PART II: SAT RESULTS

HEALTH: 1-2 **ECOTOX:** 3 **OCCUPATIONAL EXPOSURE:** 1A **CONSUMER EXPOSURE:** - **ENVIRONMENTAL RELEASES:**

Additional SAT Information:

PART III: OTHER FACTORS

a. **PRODUCTION VOLUME:** [redacted] kg/yr

b. **PROD VOL OTHER:**

c. **USE:** [redacted]

d. **REGULATORY HISTORY:** [redacted] SR MID-COURSE DISP DROP/FR
[redacted] FOCUS DROP/LETTER
[redacted] FOCUS DROP
[redacted] FOCUS DROP

e. **TEST DATA:**

f. **IMPORTED** ☐ **MANUFACTURED** ☑ **BOTH** ☐

g. **MSDS:** ☑

h. **CATEGORY:** **CATEGORY 2:** [redacted]

PART IV: SUMMARY OF SAT ASSESSMENT

CASE NUMBER: P07-0467

FATE: [redacted]

log Koc = 5.0 (P)
log fish BCF = 0.50 (P)
sorption to sludge = strong (P)
POTW removal = 0 to 50% based on uncertainty and possible sorption and biodegradation
time for complete ultimate aerobic biodegradation = weeks to months
PBT Potential: P1B1T2

HEALTH: Absorption nil thru skin, moderate thru lungs, and moderate thru GI tract based on physical/chemical properties;

concern for liver toxicity, kidney toxicity, and developmental toxicity from the pyridine moiety;
concern for irritation to mucous membranes and eyes because all of the amines are not neutralized by the HCL;
concern for lung toxicity if inhaled due to potential surfactancy;

concern for possible sensitization based analogs;

low to moderate concern for toxicity

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:
fish 96-h LC50 = 0.500 P
daphnid 48-h LC50 = 0.400 P
green algal 96-h EC50 = 0.200 P
SW algae 72-h EC50 c = 1.0 P GA72r/2
SW algae 72-h EC50 r = 2.2 M S,N
fish chronic value = 0.050 P
daphnid ChV = 0.040 P
algal ChV = 0.050 P
SW algae ChV c = 1.3 P
SW algae ChV r = 1.3 M S,N
Predictions are based on SAR-nearest analog analysis for aliphatic amines with log Kow for the [redacted]; SAR chemical class = aliphatic amine-[redacted] = [redacted] effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;
high concern for toxicity
significant mitigation of toxicity expected in the presence of 10 mg TOC/L, i.e., > 20X;
assessment factor = 10.0
concern concentration = 0.080 mg/L (ppm)

PART V: RAD RISK RATIONALE: HUMAN HEALTH

PART VI: SUMMARY OF EXPOSURE/RELEASE

Manu:
[redacted]

Proc:
[redacted]

Use:
[redacted]

PART VII: FOCUS DECISION AND RATIONALE

DISPOSITION: Drop

RATIONALE: P07-0467 was dropped from further review. Potential risks to human health were addressed by no significant exposures expected. Although concerns were high, potential risks to the environment were low based on no expected releases to water. This was an EAB Drop.

PART VIII: CCD DISPOSITION / DD

CCD:

[redacted]

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

Case #: P-07-0467	**DCN:**
SAT Date: 6/8/2007	**SAT Chair:** V. Nabholz

Submitter: [redacted]

Chemical Name:

[redacted]

CAS RN: None	**Trade Name:** None

Structure

[redacted]

Molecular Formula: [redacted]

Molecular Wt. [redacted]	**WT%<500:**	**WT%<1000:**
MP:	**BP:** >500	**Eq. Wt:**
H2O Sol (g/L): [redacted]	**V.P.** [redacted]	
Max. Prod. Volume (kg/yr): [redacted]	**Physical State:** [redacted]	

USE: Acid corrosion inhibitor (forms protective barrier on metal surfaces) for well bores and tubulars used in oil and gas recovery. The corrosion inhibitor protects machinery from strong acid (HCl, HF, formic, acetic) injected into the wells to facilitate product recovery.
P2REC: CRSS: Drop. P2 Claim. The PMN substance can be formulated to avoid using toxic substances that are used in traditional formulations, such as acetylenic alcohols, nonylphenol-based surfactants and transition metals. Also, when compared to traditional formulations, less material is required to produce the desired effect In some cases, up to half the amount of PMN-containing inhibitor is needed to provide the same amount of protection as several commercially available inhibitors.

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus Date: JUN 14 2007 **Results:** DROP

5 0 0 7 0 0 0 3 7 1 4

STRUCTURE ACTIVITY TEAM REPORT 08 June 2007 [redacted]

CASE NUMBER: **P07-0467**

P2REC: dropped at CRSS

RELATED CASES: [redacted]

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL:	1-2	3

KEYWORDS: AQUATOX-A,C, IRR-E,MM,L, LIVER, LUNG, SENS

SUMMARY OF ASSESSMENT:

FATE: [redacted]

log Koc = 5.0 (P)
log fish BCF = 0.50 (P)
sorption to sludge = strong (P)
POTW removal = 0 to 50% based on uncertainty and possible sorption and biodegradation
time for complete ultimate aerobic biodegradation = weeks to months
PBT Potential: P1B1T2
*CEB FATE: migration to ground water = negligible

HEALTH: Absorption nil thru skin, moderate thru lungs, and moderate thru GI tract based on physical/chemical properties;

concern for liver toxicity, kidney toxicity, and developmental toxicity from the pyridine moiety;
concern for irritation to mucous membranes and eyes because all of the amines are not neutralized by the HCL;
concern for lung toxicity if inhaled due to potential surfactancy;
concern for possible sensitization based analogs;

low to moderate concern for toxicity
*CEB HEALTH: Exposures to humans: inhalation, ingestion, and drinking water;

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:
fish 96-h LC50 = 0.500 P

daphnid 48-h LC50	=	0.400	P
green algal 96-h EC50	=	0.200	P
SW algae 72-h EC50 c	=	1.0	P GA72r/2
SW algae 72-h EC50 r	=	2.2	M S,N
fish chronic value	=	0.050	P
daphnid ChV	=	0.040	P
algal ChV	=	0.050	P
SW algae ChV c	=	1.3	P
SW algae ChV r	=	1.3	M S,N

Predictions are based on SAR-nearest analog analysis for aliphatic amines with [redacted]; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;
high concern for toxicity
significant mitigation of toxicity expected in the presence of 10 mg TOC/L, i.e., > 20X;
assessment factor = 10.0
concern concentration = 0.080 mg/L (ppm)
*CEB ECOTOX: All releases to surface waters with CC = 80 ppb.\

SAT Co-chair: Vince Nabholz, 564.8909

NCSAB SAT REPORT [redacted]

PMN: P-07-0467	CAS RN: None
Chemical Name: [redacted]	Analogs:
	Production Volume: [redacted]

Structure: [redacted]

[redacted]

Formula: [redacted]	Eq Wt:		
Mol Weight: [redacted]	Wt%<500:		Wt%<1000
MP:		BP: >500	VP: <0.000001
H2O Sol (g/L): [redacted]	Physical State: [redacted]		Log P: [redacted]

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	~~0.001~~	0.500	
Daphnid 48-h	~~0.021~~	0.400	
Algal 96-h	~~0.11~~	0.200	
Fish ChV	~~0.001~~	0.050	
Daphnid ChV	~~0.002~~	0.040	
Algal ChV	~~0.027~~	0.050	
BCF			

CHEMICAL CLASS:	SAR: alkNH2 – [redacted]
ECOTOX CONCERN (H) M L	CONCERN CONCENTRATION ~~0.001~~ 0.004
DATE 6/8/07	ASSESSOR:

[redacted]

SMILES : [redacted]
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: [redacted]
MOL WT : [redacted]
Log Kow:
Melt Pt:
Wat Sol:

ECOSAR v0.99h Class(es) Found

Aliphatic Amines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	Fish	14-day	LC50	0.007
Aliphatic Amines	Fish	96-hr	LC50	0.028 *
Aliphatic Amines	Daphnid	48-hr	LC50	0.004
Aliphatic Amines	Green Algae	96-hr	EC50	0.056 *
Aliphatic Amines	Green Algae	96-hr	ChV	0.045 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: none
Green algal EC50 toxicity log Kow cutoff: none
Chronic toxicity log Kow cutoff: none
MW cutoff: none

[redacted]

SMILES [redacted]
CHEM :
MOL FOR: [redacted]
MOL WT : [redacted]

---------- EPI SUMMARY (v3.12) ----------

Physical Property Inputs:
Water Solubility (mg/L): ------ Log Kow (oct-water): [redacted]
Vapor Pressure (mm Hg) : ------ Boiling Pt (deg C):
Henry LC (atm-m3/mole) : ------ Melting Pt (deg C):

Log Kow (KOWWIN v1.67 estimate) = [redacted]

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (deg C): [redacted]
Melting Pt (deg C): [redacted]
VP(mm Hg,25 deg C): [redacted]

Water Solubility estimate (WSKOW v1.41): [redacted]

Water Solubility estimate (fragments): [redacted]

Henrys Law Constant (atm-m3/mole) [HENRYWIN v3.10]:
Bond Method: 2.57E-008 Group Method: Incomplete
Henrys LC [VP/WSol estimate using EPI values]: [redacted]

Biodegradation Estimates (BIOWIN v4.02):

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
OH Half-Life = 0.041 Days (12-hr day; 1.5E6 OH/cm3)
No Ozone Reaction Estimation

Soil Adsorption (PCKOCWIN v1.66): Koc = 2.002E+007 Log Koc = 7.301

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure!

BCF estimate (BCFWIN v2.15): Log BCF = 2.502 (BCF = 317.5)

Volatilization from Water: (Henry LC = 2.57e-008 atm-m3/mole)
Half-Lives: Model River = 4.497e+004 hr, Model Lake = 4.908e+005 hr

Removal In Wastewater Treatment (percents,99% recommended maximum):
TOTAL: 93.99, Biodeg: 0.78, Sludge: 93.21, Air: 0.00

Level III Fugacity Model (conc %,half-life hr):
Air(0.0135%,0.974),Water(1.94%,900),Soil(29.4%,1.8e+003),Sediment(68.6%,8.1e+003)
Persistence Time: 3.15e+003 hr

CHEMICAL: Unknown 15:07:59 06/07/:7

MOL WT :

MOL FOR:

SMILES :

ISOC-ID: --aaaaa-ZA--AA-AA-AAAA-A-AAA-AA-AAAA

FRAG-ID: 1 2 3

H-COUNT:

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE JUN 8 2007

ATTENDEES	SIGNATURE
CHEMISTRY	
✓ Paul Bickart	
___ Diana Darling	
___ Rich Engler	
___ Greg Fritz	
___ Daniel Lin	
___ Kathy Schechter	
___ _____	
ENVIRONMENTAL FATE	
___ Bob Boethling	
✓ Wen-Hsiung Lee	
___ Laurence Libelo	
___ David Lynch	
___ Andy Mamantov	
___ _____	
HEALTH	
✓ Katherine Anitole	
✓ Michael Cimino	
✓ Steve Cragg	Steve Cragg
✓ Leonard Keifer	
___ David Lai	
✓ Jim Murphy	MEMO
___ Deborah Norris	
✓ Ronald Ward	MEMO
✓ Yin Tak Woo	
___ _____	
___ _____	
ENVIRONMENTAL EFFECTS	
✓ Gordon Cash	MEMO
___ Vince Nabholz	
___ Maggie Wilson	
___ _____	
SAT CHAIR/OTHER	
___ Rebecca Jones	
___ Leonard Keifer	
✓ Vince Nabholz	
___ Jim Kwiat	
___ _____	